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Hanford Tank Farms Vadose Zone

Effects of Differing Source Distributions on Spectral Shape Factors for Contaminant Logging at the Hanford Site

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1.0 Abstract

Computer radiation transport modeling calculations were performed in the past to simulate passive gamma-ray logs of selected non-uniform gamma-ray source distributions. Those studies led to a spectral shape factor analysis that is presently used by data analysts to determine spatial distributions of gamma-ray emitters from borehole logs from the Hanford Tank Farms. Some variations in the radial (horizontal) distribution of sources were explicitly modeled in the earlier studies, but axial (vertical) variations were not.

This report describes extensions of the computer model that were created and used to simulate effects on the spectral shape factors of axial variations in the distribution of cesium-137 (^{137}Cs) source, and, in addition, radial distribution variations that were not considered in the earlier studies. Three types of ^{137}Cs distribution were modeled: (1) source of uniform concentration distributed between an outer cylindrical surface of variable radius with its cylinder axis coincident with the borehole axis, and an inner cylindrical surface of fixed radius that coincided with the outer wall of the borehole casing (the difference in radii between the two cylindrical surfaces determined the thickness of the source layer), (2) source of uniform concentration distributed in a thick horizontal tabular zone, and (3) source of uniform concentration distributed in a thin horizontal tabular zone.

Because spectral shape factors are calculated using spectral energy ranges in which Compton scattering is the dominant interaction of gamma rays with matter, the shape factor effects could be qualitatively predicted from the understanding of how the Compton continuum would be affected by changes in the source distribution. Three expected behaviors of the spectral shape factors were confirmed by the computer simulations. For the source confined to the zone bounded by the two cylindrical surfaces, the 661.6-keV spectral peak intensity and the spectral shape factor named CsSF1 both initially increased as the (radial) thickness of the zone increased. As the zone thickness expanded, the peak intensity and shape factor did not increase indefinitely, but both attained limiting values at a zone thickness of about 15 centimeters (cm). For the thick tabular source zone, CsSF1 increased as the axial separation between the gamma-ray detector and the horizontal zone boundary grew. For the simulated log through a thin tabular source zone, the values of CsSF1 in relation to depth were anticorrelated with the depth profile of ^{137}Cs concentration.

2.0 Introduction

The U.S. Department of Energy's (DOE) Grand Junction Office (DOE-GJO) is gathering and interpreting data to construct the first comprehensive data base on the identities and distributions of gamma-ray-emitting radionuclides in the vadose zone beneath the tank farms at the Hanford Site. This baseline characterization of the gamma-ray emitters, which are constituents of radioactive wastes around the single-shell tanks in the Hanford Tank Farms, was requested by the DOE Richland Operations Office (DOE-RL). The baseline data are acquired by logging existing boreholes with high-resolution passive spectral gamma-ray logging systems (SGLSs).

The most elementary analysis of high resolution spectral gamma-ray log data utilizes only the energies and intensities associated with peaks in the gamma-ray spectra. Energies are the basis for identification of the gamma-ray sources, and intensities, properly corrected for system deadtime, borehole casing, and other effects, are translated, via the logging system calibration, into source concentrations.

The logging system calibrations are derived from spectra recorded by logging large blocks of material within which gamma-ray sources exist in known concentrations and uniform distributions. Therefore, the application of the calibration to the calculation of a source concentration carries the assumption that the source is uniformly distributed in a large volume of medium surrounding the sonde. That a gamma-ray source in the subsurface is uniformly distributed is always open to question, but the assumption is especially strained in the Hanford Tank Farms, where the borehole drilling method and other factors have probably encouraged some deposition of contaminants in non-uniform distributions. Hanford log data indicate that a likely non-uniform distribution is the "casing distribution" in which the contaminant exists primarily as a layer on the outer casing wall. This distribution probably resulted most often from downward infusion ("dragdown"), in which materials from a contaminated zone were carried to uncontaminated depths as the casing was advanced during the (cable tool) borehole drilling. A less likely, but possible, mechanism for this contaminant distribution is deposition on an installed casing by meteoric water. Water presumably acquired contaminants when flowing over a contaminated ground surface or through a contaminated subsurface zone, then deposited those contaminants on casings that acted as conduits for water in the subsurface.

Wilson (1997) realized that the elementary data analysis would yield inaccurate concentrations if contaminants were present in a borehole casing distribution or other non-uniform configuration. In response, Wilson (1997) and Wilson et al. (1998) showed that certain non-uniform source distributions could be distinguished from uniform source distributions with numerical factors that exploited measurable differences in spectral shapes. Guided by experiments and simulations of the passive gamma-ray measurements with the MCNP (Briesmeister 1993) Version 4.A Monte Carlo radiation transport code, Wilson (1997) defined several "shape factors" that can be calculated and used to infer the distributions of gamma-ray sources. The two shape factors discussed in this report are named CsSF1 and SF2. CsSF1, or cesium shape factor 1, was defined by Wilson as the ratio of the counts in the spectral continuum between 60 and 650 keV to the counts in the full energy cesium peak at 661.6

keV. SF2, or shape factor 2, was defined as the ratio of the counts in the spectral continuum between 60 and 350 keV to the counts in the continuum between 350 and 650 keV.

Wilson (1997, 1998) calculated values of CsSF1 and SF2 for several configurations of ^{137}Cs, including a layer on the inner casing surface, a layer on the outer casing surface, a uniform distribution in the formation surrounding the borehole, and a few distributions in the formation radially distant from the borehole. A shape factor analysis method based on Wilson's values is one of the techniques used currently to infer the distributions of gamma-ray sources.

This report describes the behaviors of the shape factor parameters CsSF1 and SF2 for ^{137}Cs distributed in zones radially close to the borehole. These distributions were modeled to assess the "radius of investigation" of the passive spectral gamma-ray measurements. In addition, simulations of thick and thin tabular source zones at various axial distances from the gamma-ray detector were undertaken to determine shape factor trends associated with movement of the sonde toward or away from tabular zones.

All of the results in this report were derived from MCNP simulations of the logging measurements. Some of the shape factors that were calculated for cases with significant axial distances between detector and source may be inaccurate to a minor, but unknown, degree due to well known difficulties ("deep penetration" problems) of calculating accurate gamma-ray fluxes incident on a detector when the separation between detector and source is large (many mean free paths). Such inaccuracies do not, however, detract from the results in this report because the results are not intended to be used to calculate concentrations of sources distant from the detector. The results show trends exhibited by CsSF1 and SF2 as source distributions change, and these trends can be used by data analysts to deduce the most plausible distribution of non-uniform sources that will account for log data.

3.0 Computer Simulations

3.1 General Features of the Computer Model

The starting point for the study described in this report was Wilson's (1997) MCNP model for spectral shape factor investigations. The geometry and materials specifications in the MCNP input file defined a circular cylindrical borehole cased with a 0.28-inch (in.)-thick steel pipe with an outer diameter of 6.25 in. This type of pipe was typically used as borehole casing at Hanford. The model placed no grout or air gap between the casing and the surrounding formation; this also replicated the typical borehole configuration at Hanford. The formation around the borehole was modeled as SiO_2 with a density of 1.8 grams per cubic centimeter (g/cm^3) and a moisture content of 3 percent by mass. The geometry and materials inputs also simulated components of the type of sonde used for the DOE-GJO logging in the Hanford Tank Farms. The model included the sonde housing, the high purity germanium detector, and the parts of the cryostat system that would affect the gamma-ray fluxes incident on the detector surface. These features are depicted in section view in Figure 1.

The sonde was fully eccentered in the borehole, as shown in Figure 1. The borehole, borehole casing, and formation were cylindrically symmetric about the vertical line that passes through the zero on the radial scale.

It should be noted that the outer radius of the formation and the vertical extent of the formation were model variables; these quantities were not fixed at 20 cm and 40 cm, as Figure 1 might imply.

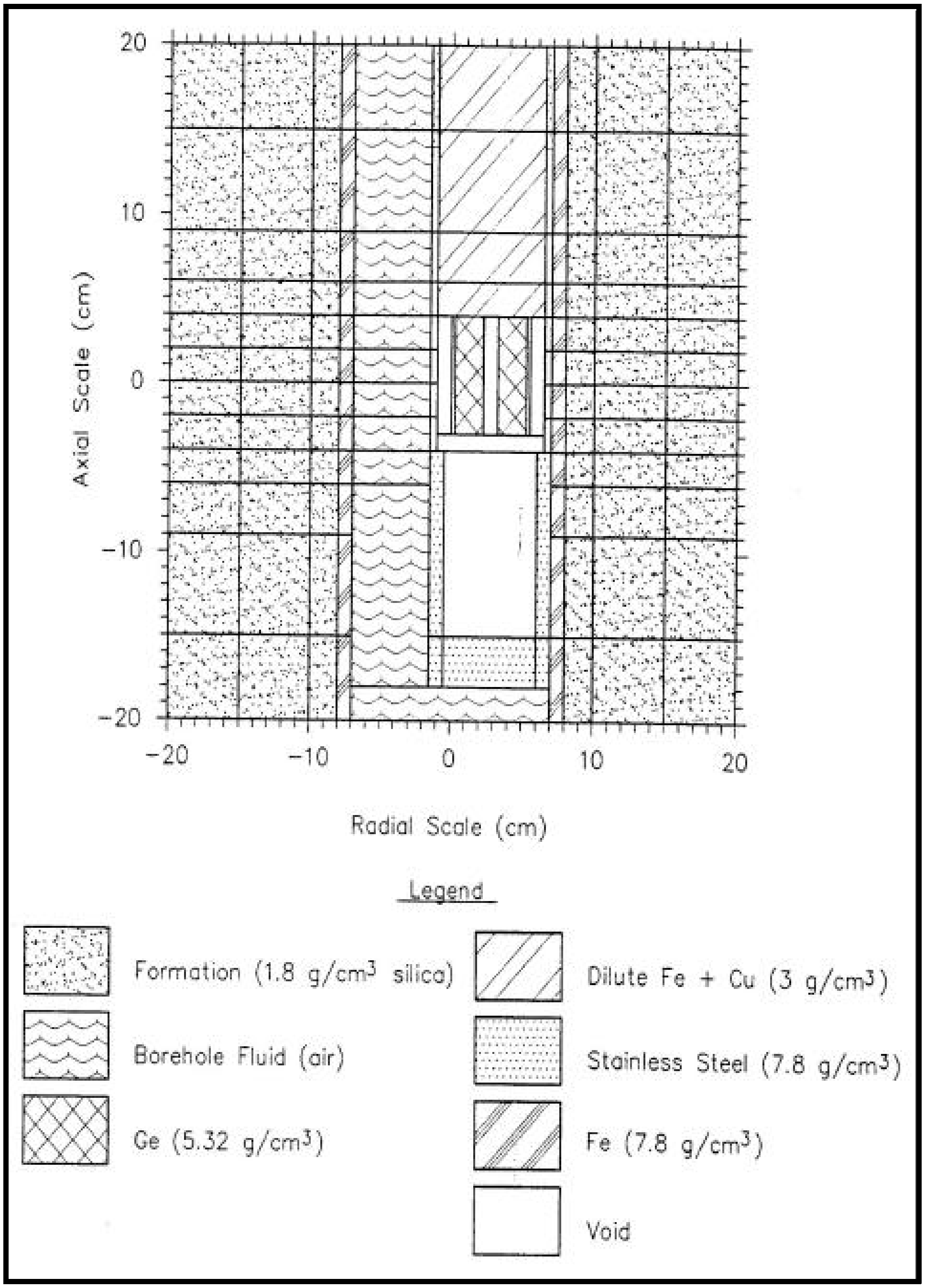

Figure 1. Section View of the Principal Features of the MCNP Model

The MCNP "type f8" pulse height tally was used, meaning that the MCNP outputs were pulse height spectra (instead of, for example, flux spectra). The f8 tally was recently introduced in Version 4A, and it should be noted that it hasn't been tested as extensively as the older MCNP tally types. The pulse height spectra had statistical uncertainties because MCNP, like all Monte Carlo programs, simulates photon traverses and interactions in the model materials by statistical methods. Statistical uncertainties in an MCNP output tally can generally be reduced by increasing the number of source photons in the program run. For the study described in this report, pulse height spectra with high levels of precision were produced by running each MCNP simulation with a large number (45 million) of source photons.

3.2 Computer Model for Radius of Investigation Determination

To determine the radius of investigation of the gamma-ray measurements, MCNP was configured to simulate ^{137}Cs sources distributed within layers of various thicknesses wrapped around the borehole. This was accomplished for each run by geometry and source specifications that distributed the source within the part of the formation that lays between two collinear circular cylindrical surfaces. The inner surface coincided with the outer edge of the borehole casing, and the outer surface was a circular cylinder that defined the outer edge of the source-bearing part of the formation. In other words, if the z cylindrical coordinate axis coincided with the borehole axis, and the r coordinate had the value R on the outer edge of the borehole casing (R = 6.25 in.), then the source occupied a volume defined by R < r < R + ? R, where ? R was the layer thickness. The outer radial boundary of the model “universe” was set at 75 cm. In the vertical direction, the model formation extended from 40 cm below the center of the detector to 40 cm above. These vertical dimensions far exceeded the mean free path of the 661.6-keV gamma ray of ^{137}Cs in the formation (about 7 cm); therefore, the vertical extent of the formation was effectively infinite with respect to radiation transport.

MCNP was executed with values of ? R equal to 1, 3, 5, 8, 10, 15, 20, 25, 30, 35, 40, 45, and 50 cm. In each MCNP output, the peak pulse height tally was expressed in relation to the “concentration”(number of source photons per unit volume), but because the number of source photons was constant (45 million) and the volume occupied by the source increased as ? R increased, the concentration was inversely related to the source volume. To make all of the tallies relative to the same concentration, each tally was multiplied by (V/V_0), where V_0 was the smallest source volume (corresponding to ? R = 1 cm), and V was the volume for the particular tally with ? R > 1 cm.

An alternative to the adjustment of tallies by volume ratios would have been maintenance of a constant source concentration by increasing the number of source photons in direct proportion to each increase in source volume. This was not done because the computer time for an MCNP run is directly proportional to the number of source photons, and the run times would have been unjustifiably long for the larger source volumes. Furthermore, when the source volume is large, the many photons that originate at great distances from the detector consume computer processing time, but contribute little to the tally.

Because the source concentration decreased as the source volume increased, the number of photons that contributed to the tally decreased as the source volume increased. Consequently, the statistical fluctuations in the tallies increased with increasing source volume. Qualitative observations of the statistical fluctuations in the calculated pulse height spectra indicated that the fluctuations were not large enough to cast doubt on the conclusions cited in this report.

3.3 Computer Model for Effect on Shape Factors of Logging Past a Thick Source Zone

The effect on CsSF1 and SF2 of logging through a thick source layer was simulated with a set of MCNP runs with varying distances between the detector (which was always below the source layer) and the lower boundary of a large zone with a uniform distribution of ^{137}Cs. The zone containing the ^{137}Cs was bounded by two horizontal planes 50 cm apart and a circular cylinder with a radius of 50 cm from the borehole center. The cylinder axis was coincident with the cylinder axis of the borehole.

Five (axial) distances between the center of the detector and the plane at the lower boundary of the source zone were modeled: 0, 0.01, 5, 10, and 15 cm.

3.4 Computer Model for Effect on Shape Factors of Logging Past a Thin Source Zone

The effect on CsSF1 and SF2 of logging through a thin source layer was simulated by the same MCNP techniques as used for the thick source zone, except the thickness of the zone was 2.54 cm.

Twelve (axial) distances between the center of the detector and the center of the source zone were modeled: 0, 0.01, 5, 10, 15, 20, 25, 30, 35, 40, 45, and 50 cm.

4.0 Results

4.1 Radius of Investigation

The MCNP results for the radius of investigation study are tabulated in Table 1 and are plotted in Figures 2, 3, and 4.

Table 1. MCNP Results for the Radius of Investigation Study

Radial Extent ? R (cm)	Source Volume (cm^3)	Source Scale Factor V/Vo	661.6-keV Spectral Peak Intensity (counts)	Adjusted 661.6-keV Peak Intensity (counts)	Spectral Continuum 60 to 650 keV (counts)	Low Continuum 60 to 350 keV (counts)	High Continuum 350 to 650 keV (counts)	CsSF1	SF2
1	1635.03	1.00	0.00158	0.00158	0.01134	0.00804	0.00290	7.17	2.77
3	5479.62	3.35	0.00119	0.00399	0.00949	0.00679	0.00237	7.97	2.86
5	10090.30	6.17	0.00091	0.00564	0.00804	0.00579	0.00197	8.84	2.94
8	18442.60	11.28	0.00065	0.00735	0.00633	0.00460	0.00151	9.74	3.05
10	24968.30	15.27	0.00053	0.00806	0.00544	0.00397	0.00129	10.26	3.08
15	44634.10	27.30	0.00034	0.00928	0.00382	0.00281	0.00088	11.24	3.19
20	69087.80	42.25	0.00023	0.00973	0.00276	0.00204	0.00063	12.00	3.24
25	98329.20	60.14	0.00016	0.00981	0.00207	0.00153	0.00047	12.94	3.26
30	132358.00	80.95	0.00012	0.00995	0.00160	0.00118	0.00036	13.33	3.34
35	171175.00	104.69	0.00010	0.00996	0.00125	0.00118	0.00036	12.50	3.27
40	214780.00	131.36	0.00008	0.01001	0.00100	0.00075	0.00022	12.50	3.41
45	263173.00	160.96	0.00006	0.01033	0.00083	0.00061	0.00019	13.83	3.21
50	316353.00	193.49	0.00005	0.01024	0.00069	0.00051	0.00015	13.80	3.40
60	437077.00	267.32	0.000037	0.00989	0.00049936	0.0003728	0.0001084	13.28	3.44
70	576952.00	352.87	0.000028	0.00988	0.000377	0.000282	0.000082	13.46	3.44
80	735979.00	450.13	0.000023	0.01035	0.000299	0.000223	0.000065	13.0	3.43

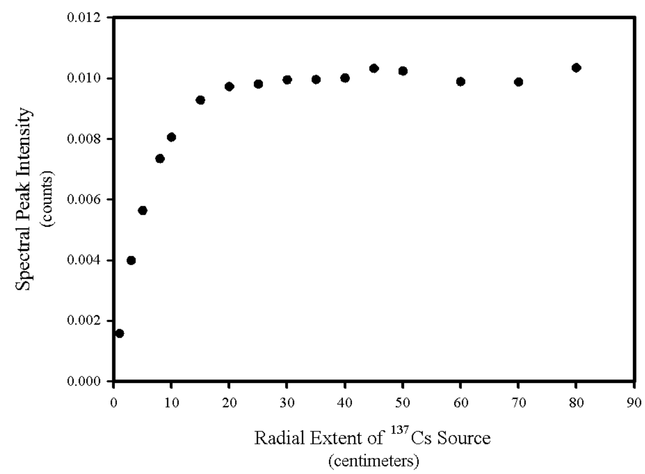

Figure 2. Intensity of the Adjusted 661.6-keV Spectral Peak in Relation to the Radial Extent of the ^{137}Cs Source

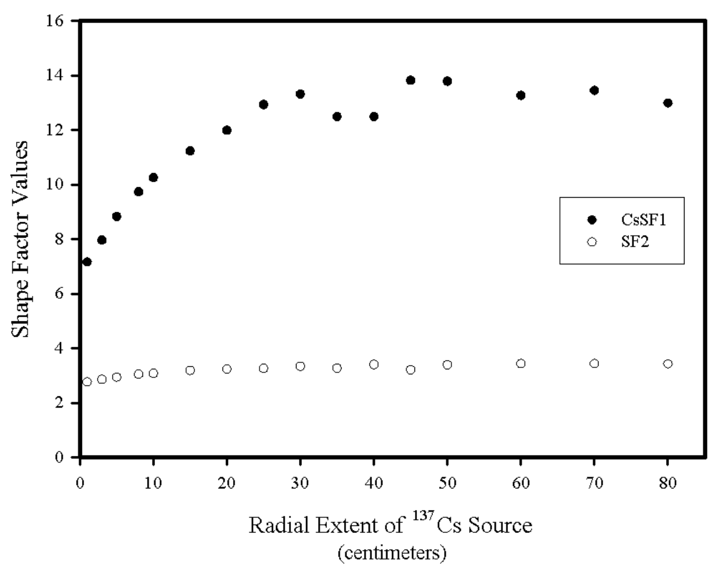

Figure 3. Shape Factors in Relation to the Radial Extent of the ^{137}Cs Source

Figures 2 and 3 indicate that the 661.6-keV peak intensities and the CsSF1 values both rise initially as the radial extent of the ^{137}Cs-bearing medium expands, and as the radial extent increases further the peak intensities and shape factors approach asymptotic limits. The "statistical noise" in the plots is a consequence of the fact that the Monte Carlo method generates solutions statistically instead of analytically. The changes in peak intensities and shape factors that accompany changes in the source distribution are fully consistent with expectations based on Compton scattering of gamma rays within the source medium. The peak intensity reaches 90 percent of the asymptotic limit when the source extends to about 14.8 cm (5.83 in.) beyond the outer surface of the borehole casing, and CsSF1 reaches 90 percent when the source extends to about 15 cm.

These results indicate that the "radius of investigation" of the gamma-ray log and the CsSF1 shape factor can be taken to be about 15 cm or 5.8 in. for gamma rays with energies near 660 keV. The radius of investigation is larger for gamma rays with higher energies, and smaller for gamma rays with lower energies.

In contrast to CsSF1, SF2 is nearly insensitive to the radial extent of the source-bearing medium.

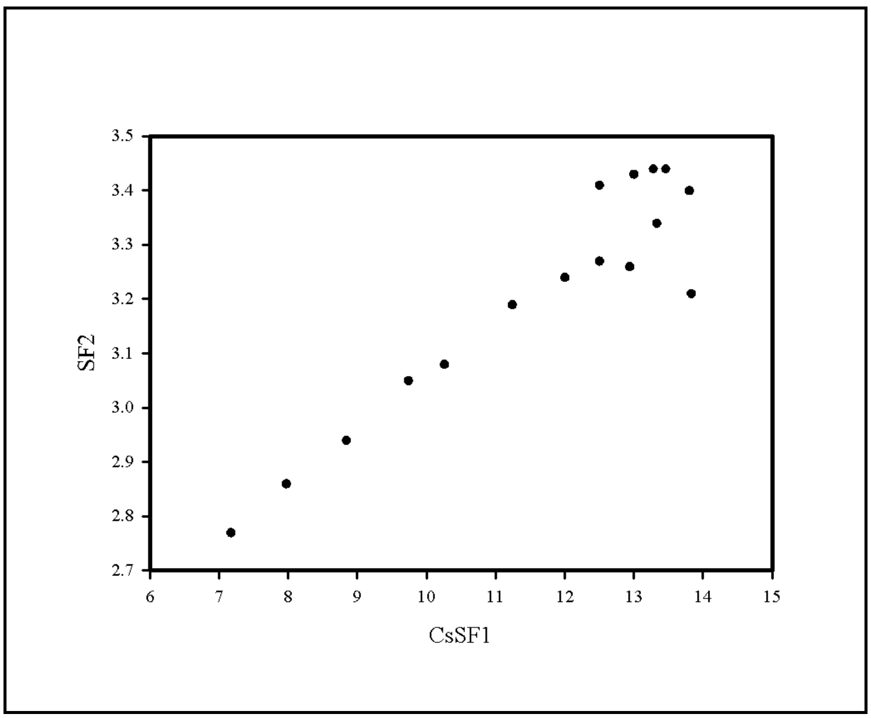

Figure 4. SF2-CsSF1 Crossplot for the Radial Extent Source Model

The points in Figure 4 trace a "trend line" in a cross plot of SF2 versus CsSF1. The trend line indicates the normal behavior of SF2 in relation to CsSF1 when ^{137}Cs is the only photon source in the formation and the outer boundary of the source moves radially outward from the borehole. The upper end of the trend line has a cluster of points corresponding to the set of nearly identical CsSF1 values that the model yielded when ? R exceeded about 25 cm and all of the CsSF1 values were close to the asymptotic limit.

4.2 Effect of Logging Past a Thick Source Zone

Peak intensities and shape factors were calculated for a set of ^{137}Cs spectra that simulated logging measurements at various axial distances downward from the boundary of a 50-cm-thick (measured vertically) tabular zone in which the ^{137}Cs concentration was uniform.

As expected, the intensity of the spectral peak for the 661.6-keV gamma ray decreased as the distance from the source zone increased. As the peak intensity diminished, the relative intensity in the Compton continuum increased, leading to an increase in CsSF1 as the axial distance increased.

The calculated results are tabulated in Table 2. The plot in Figure 5 depicts the decrease in spectral peak intensity with increasing axial distance, and the plot in Figure 6 shows the corresponding increase in CsSF1.

The plots in Figures 5 and 6 show the behaviors of peak intensity and CsSF1 as the sonde moves away from a thick zone in the downward direction. If the sonde moved upward from the thick zone the same qualitative effects would have been observed. For upward movement, the peak intensities and CsSF1 values might not exactly match their counterparts for downward movement because the spectra are affected by photon scattering and absorption within components of the sonde near the detector, and the part of the sonde that lies below the midpoint of the detector is not a mirror image of the part that lies above the detector midpoint.

Table 2. MCNP Results for the Thick Source Zone Study

Axial Distance between Zone Boundary and Center of Detector (cm)	Zone Volume (cm^3)	661.6-keV Spectral Peak Intensity (counts)	Spectral Continuum 60 to 650 keV (counts)	Low Continuum 60 to 350 keV (counts)	High Continuum 350 to 650 keV (counts)	CsSF1
0	3.92699e+05	3.12e-05	0.00042581	0.0003198	0.000094	13.7215
0.01	3.92699e+05	3.23778e-05	0.0004308	0.0003182	0.000097	13.3116
5.01	3.92699e+05	1.59778e-05	0.0002713	0.0002025	0.000059	16.961
10.01	3.92699e+05	6.7778e-06	0.00015804	0.00011996	0.000032	23.3174
15.01	3.92699e+05	2.95556e-06	0.0000884	0.00006 85	0.000017	29.7744

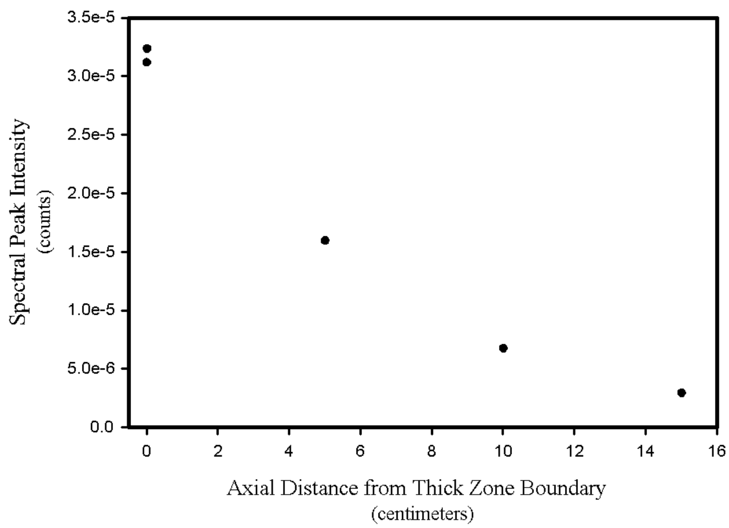

Figure 5. Peak Intensity in Relation to Distance from a Thick Source Zone

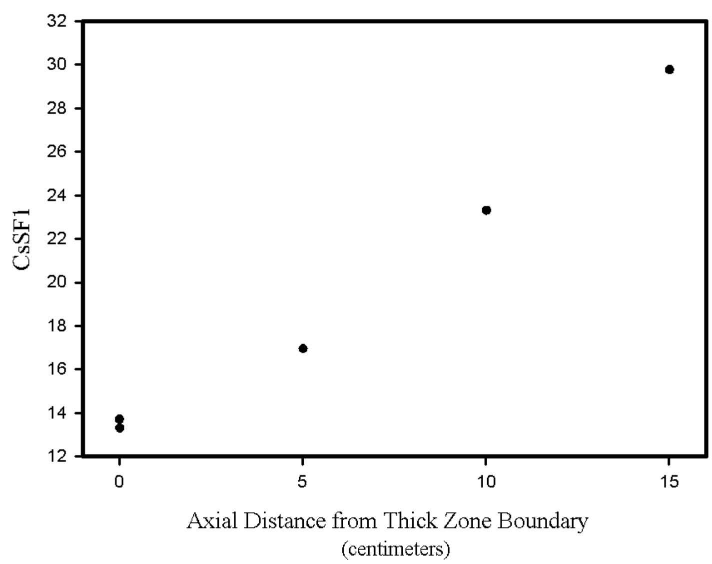

Figure 6. Shape Factor CsSF1 in Relation to Distance from a Thick Source Zone

4.3 Effect of Logging through a Thin Source Zone

Peak intensities and shape factors were calculated for a set of ^{137}Cs spectra that simulated logging measurements at various axial distances downward from the center of a tabular 2.54-cm-thick (measured vertically) zone within which the concentration of ^{137}Cs was modeled as uniform.

The intensity of the spectral peak for the 661.6-keV gamma ray decreased as the distance from the source zone increased. As the peak intensity diminished, the relative intensity in the Compton continuum rose, leading to an increase in CsSF1 as the axial distance increased.

The calculated results are tabulated in Table 3. The plot in Figure 7 depicts the decrease in spectral peak intensity with increasing axial distance, and the plot in Figure 8 shows the corresponding increase in CsSF1.

For reasons explained in Section 4.2, the general behavior of the peak intensity and the shape factor CsSF1 would be nearly the same if the sonde had been modeled as moving upward from the source zone.

Table 3. MCNP Results for the Thin Source Zone Study

Axial Distance Between Center of Zone and Center of Detector (cm)	Source Zone Volume (cm^3)	661.6-keV Peak Intensity (counts)	Spectral Continuum 60 to 650 keV (counts)	Low Continuum 60 to 350 keV (counts)	High Continuum 350 to 650 keV (counts)	CsSF1
centered	199490	172.6e-6	1.708e-3	1.237e-3	409.1e-6	9.89
0.01	199490	172e-6	1.713e-3	1.245e-3	407.5e-6	9.96
5	199490	105.9e-6	1.289e-3	944.3e-6	296.8e-6	12.17
10	199490	46.89e-6	775.8e-6	580.3e-6	168.9e-6	16.55
15	199490	19.51e-6	452.4e-6	342.1e-6	93.8e-6	23.18
20	199490	9.467e-6	248.2e-6	190.4e-6	49.02e-6	26.22
25	199490	4.111e-6	141e-6	110e-6	26e-6	34.3
30	199490	1.444e-6	78.62e-6	61.96e-6	13.91e-6	54.43
35	199490	7.556e-6	43.53e-6	34.87e-6	6.978e-6	57.61
40	199490	3.556e-6	25.13e-6	19.76e-6	4.444e-6	70
45	199490	155.6e-9	14.64e-6	11.64e-6	2.422e-6	94.11
50	199490	66.67e-9	7.6e-6	6.2e-6	1.2e-6	114

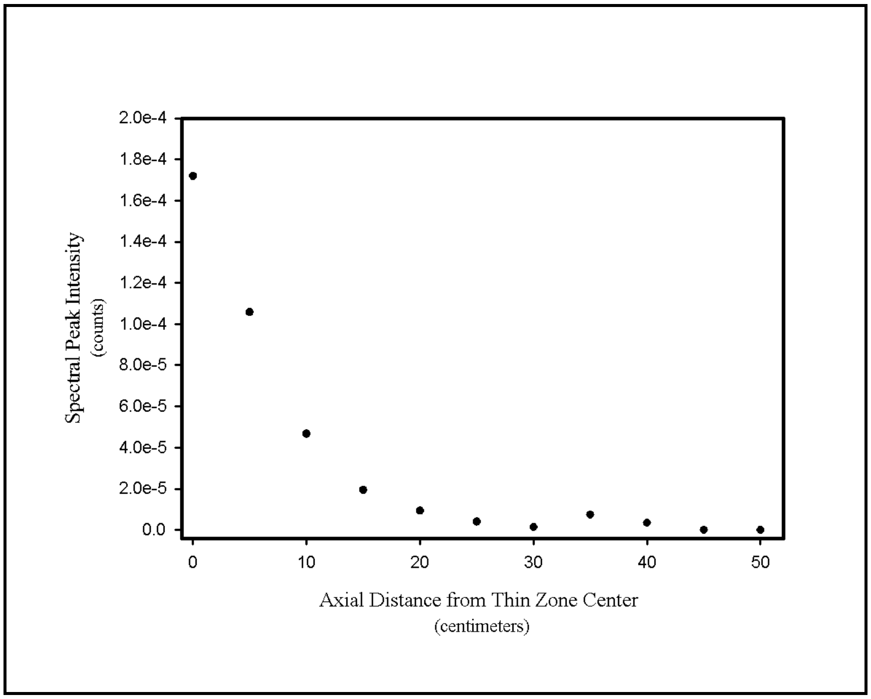

Figure 7. Spectral Peak Intensity in Relation to Distance from a Thin Source Zone

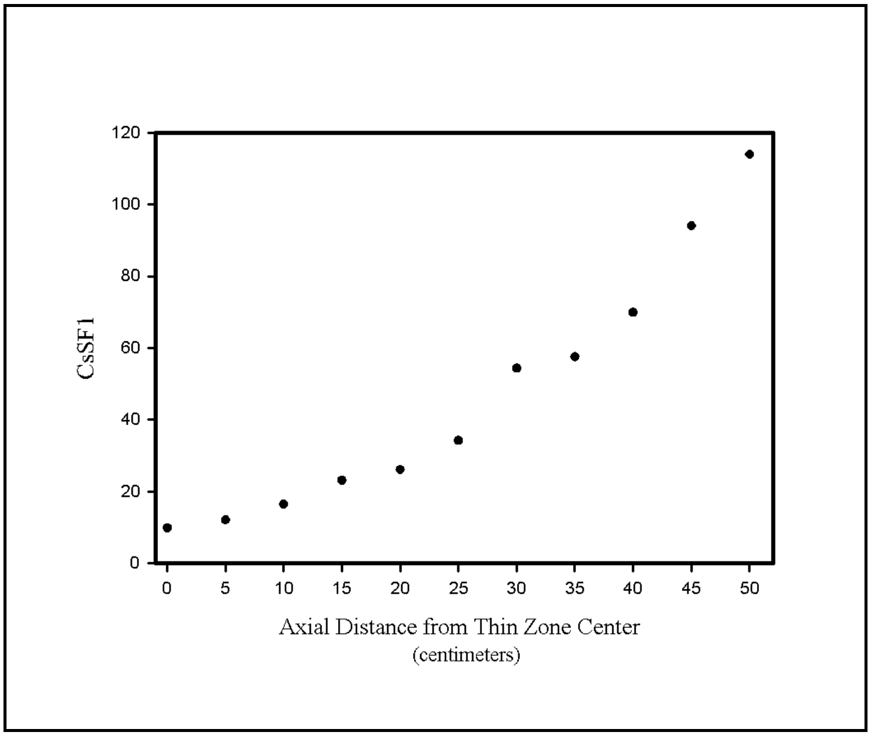

Figure 8. Shape Factor CsSF1 in Relation to Distance from a Thin Source Zone

5.0 Conclusions

This report documents an assessment of the "radius of investigation" of the passive spectral gamma-ray measurements and an investigation of the effects on CsSF1 of variations in source-to-detector separation and gamma-ray source distribution in the axial dimension.

The studies were based entirely on MCNP simulations of the logging measurements. There were probably some inaccuracies in the spectra that were simulated by computer models in which significant axial distances between detector and source existed. Such inaccuracies would have stemmed from problems ("deep penetration") that are known to afflict radiation fluxes calculated at significant distances from a radiation source. Such inaccuracies can probably be ignored because the results presented in this report are not intended to be used to calculate source concentrations. The results show how SF2 and CsSF1 behave as ^{137}Cs source distributions change, and these trends can be used by data analysts for qualitative interpretation of log data.

Wilson (1997) and Wilson et al. (1998) showed that elevated values of CsSF1 can be associated with sources that are radially distant from the borehole. The new findings indicate that a steady increase in CsSF1 that accompanies the movement of the sonde away from a thick source zone should usually be interpreted as the normal behavior of CsSF1 and not necessarily as an encounter with a second, but radially distant, zone. Likewise, an increase in CsSF1 on either side of a thin source zone (i.e., an anti-correlation of CsSF1 with source concentration) should not necessarily be interpreted as a distant source in combination with a thin stringer that reaches the borehole casing.

Of course, the distribution of contaminants in the subsurface is mostly unpredictable, and it is always possible that the borehole passes, for example, through a thick or thin contaminant zone and also near another contaminated zone that doesn't contact the borehole casing. Because uncountable combinations of source configuration are possible, the data analyst should always rely on experience and understanding of physical principles, and should not allow sound judgement to be replaced by a set of inflexible rules.

6.0 References

Briesmeister, J.D. (ed.), 1993. *MCNP--A General Monte Carlo N-Particle Transport Code, Version 4A*, La-12625 (manual), Los Alamos National Laboratory, Los Alamos, New Mexico.

Wilson, R.D., 1997. *Spectrum Shape-Analysis Techniques Applied to the Hanford Tank Farms Spectral Gamma Logs,* GJO-96-13-TAR, prepared for the U.S. Department of Energy by MACTEC Environmental Restoration Services, May 1997.

Wilson, R.D. 1998. *Enhancements, Validations, and Applications of Spectrum Shape-Analysis Techniques Applied to Hanford Tank Farms Spectral Gamma Logs*, GJO-97-25-TAR GJO-HAN-15, prepared for the U.S. Department of Energy by MACTEC Environmental Restoration Services, January 1998.

Wilson, R.D., C.J. Koizumi, J.E. Meisner, and D.C. Stromswold, 1998. "Spectral Shape Analysis for Contaminant Logging at the Hanford Site," *IEEE Transactions on Nuclear Science*, Vol. 45, No. 3, June 1998.